The University of Tennessee

Energy Efficient Thermal Management of Natural Gas Engine After treatment Via Active Flow Control

Principle Investigators

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COOPERATIVE AGREEMENT DE-FC26-02NT41609

Awarded (10/01/2002, 36 Month Duration)

$750,000 Total Contract Value ($600,000 DOE)

Project Objectives

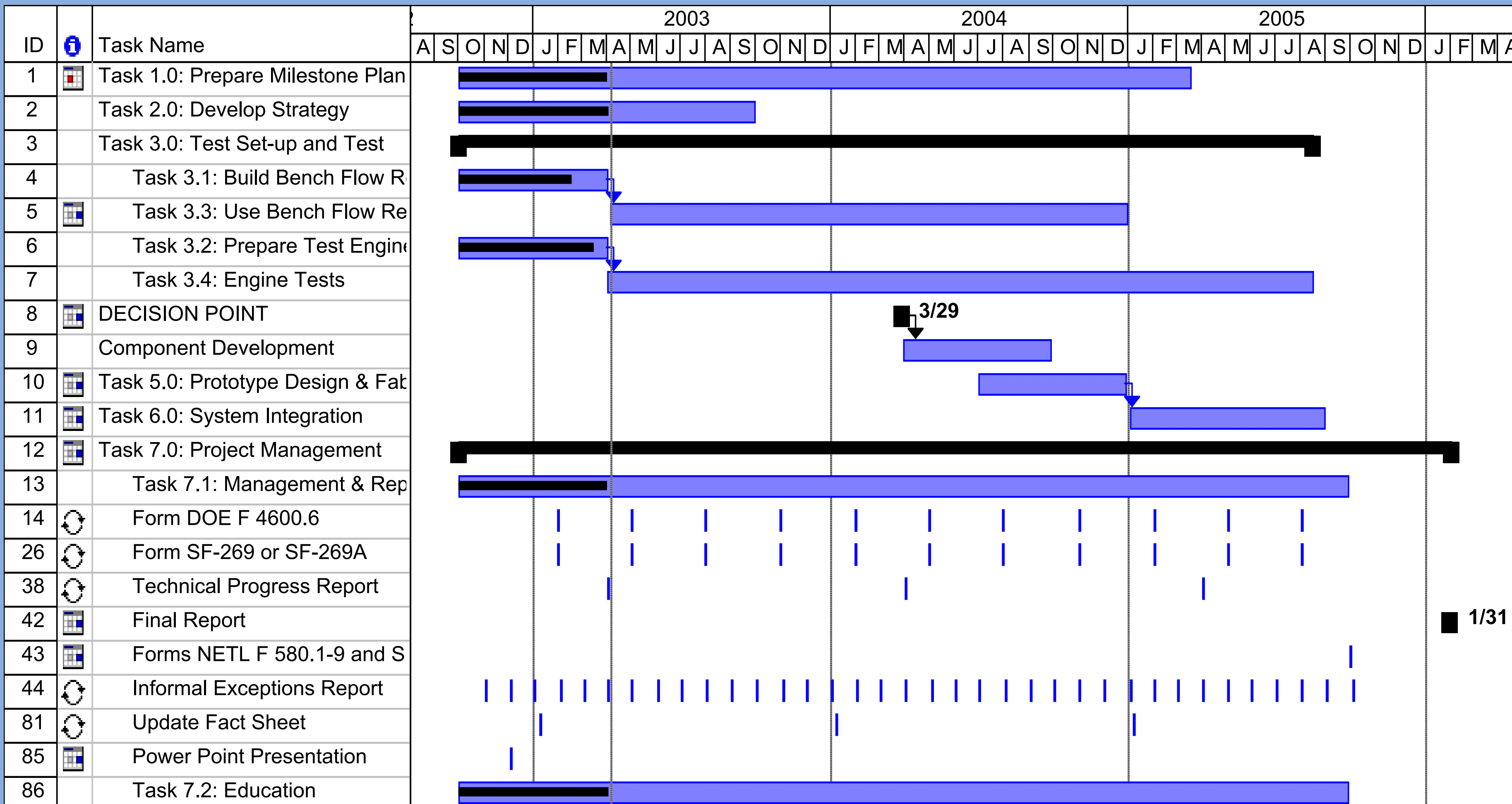
Objectives

- Reduce NO_x and CH_4 emission by 95% from lean burn natural gas engines
- Reduce supplemental fuel use by 80%

Technical Approaches

- Partial flow restriction for regeneration and desulfurization of LNT
- Alternating between regeneration and absorption for LNT
- Periodic flow reversal for oxidation catalyst
- Supplemental fuel injection for regeneration and desulfurization of LNT and for maintaining light off of oxidation catalyst

Project Schedule



Accomplishments

Constructing a bench-flow reactor system

- NO_x absorbing catalyst reactor
- Reverse flow oxidation catalyst reactor
- Water vapor generator
- Gas preheater
- National Instruments LabVIEW – based data acquisition system

Learning to use FEMLAB to obtain solutions for transient 1-D reverse-flow oxidation catalyst

- Temperature profile
- Optimum cycling frequency
- Conversion efficiency

Engine test cell at National Transportation Research Center

- Engine installation complete
- Emissions bench and data acquisition system complete
- Fire Protection Engineering approval imminent

Literature survey

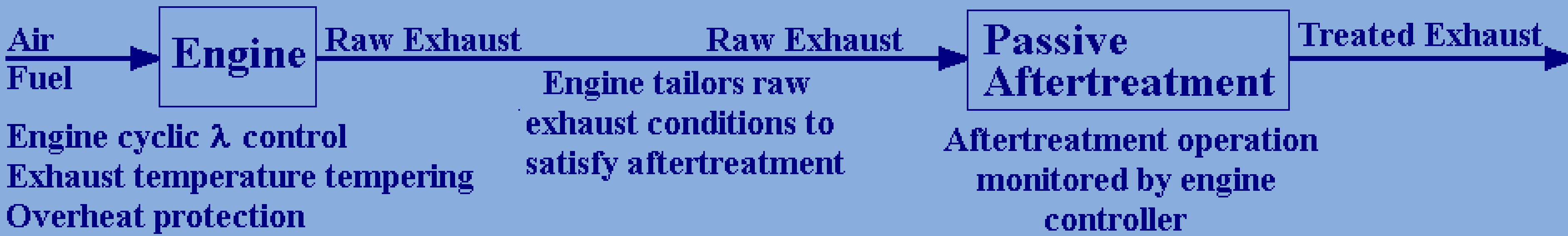
- NO_x absorbing catalyst
- Oxidation catalysts
- Emissions from natural gas engines

Technical Approaches and Results

Exhaust aftertreatment may employ passive or active control strategies

Passive Aftertreatment

- Passive control in catalytic converter
- Active control in engine fuel management



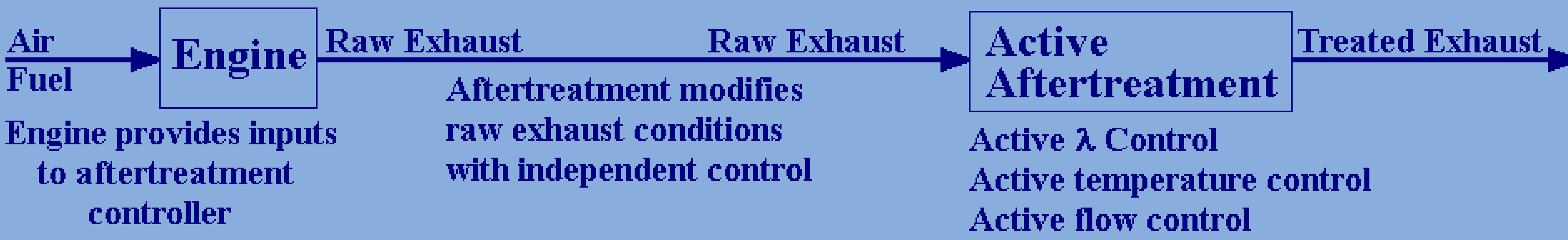
Passive Control of Exhaust Aftertreatment

Disadvantages

- Poor control of HC and CO emissions
- High penalty of fuel economy
- Power output fluctuations during rich excursions

Active Aftertreatment

- Active control in catalytic converter
- Passive control in engine fuel management



Active Control of Exhaust Aftertreatment

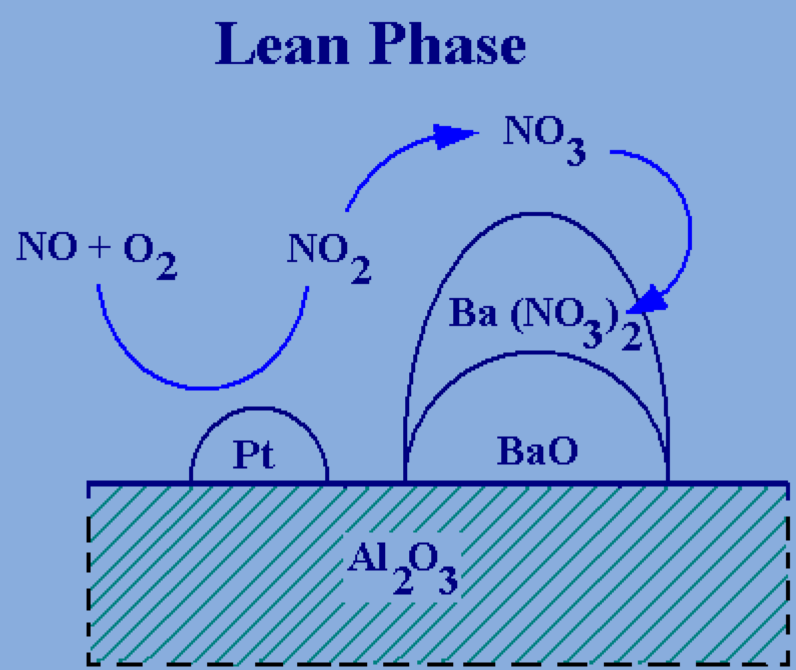
Advantages

- Energy efficient
- Rich fuel pulses are generated within individual catalysts
- Engine optimization achieved without compromising individual catalyst

Active aftertreatment control is proposed in the present investigation

NO_x Absorbing Catalyst

NO_x absorbing catalyst stores NO_x under lean conditions and reduces it during rich conditions



Lean Phase

- Oxidation of NO to NO_2

$$2NO + O_2 \longrightarrow 2NO_2$$

- NO_2 storage

$$2NO_2 + BaO + (1/2)O_2 \longrightarrow Ba(NO_3)_2$$

NO_x Absorbing Catalyst

Rich Phase

Decomposition of NO_3 with CO

$Ba(NO_3)_2 + CO \longrightarrow BaO + 2NO_2 + CO_2$

Decomposition of NO_3 with H_2

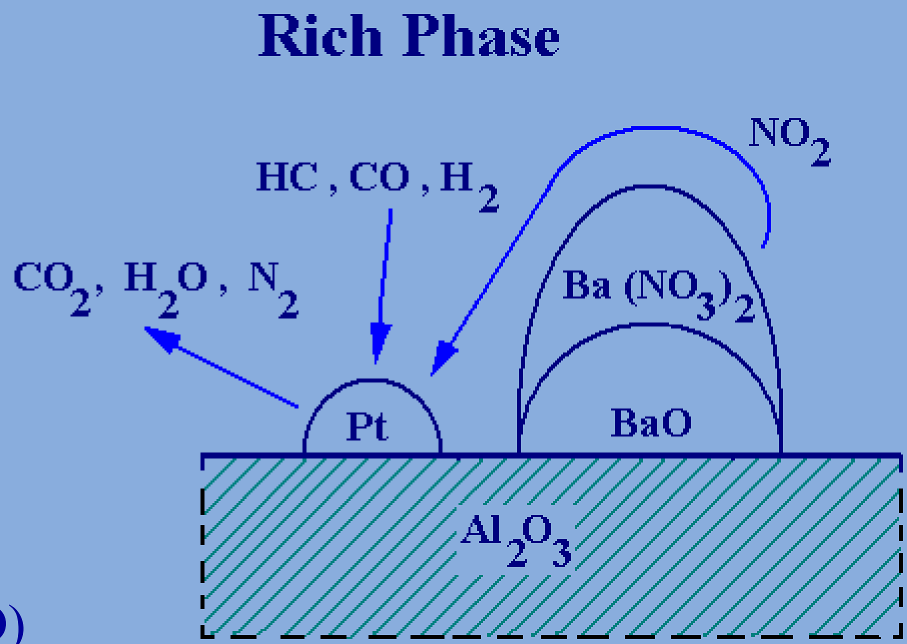
$Ba(NO_3)_2 + H_2 \longrightarrow BaO + 2NO_2 + H_2O$

NO_2 reduction by three-way principle

$NO_2 + CO \text{ (or } H_2) \longrightarrow NO + CO_2 \text{ (or } H_2O)$

$NO + CO \text{ (or } H_2) \longrightarrow (1/2)N_2 + CO_2 \text{ (or } H_2O)$

Similar reduction and decomposition steps take place with hydrocarbon

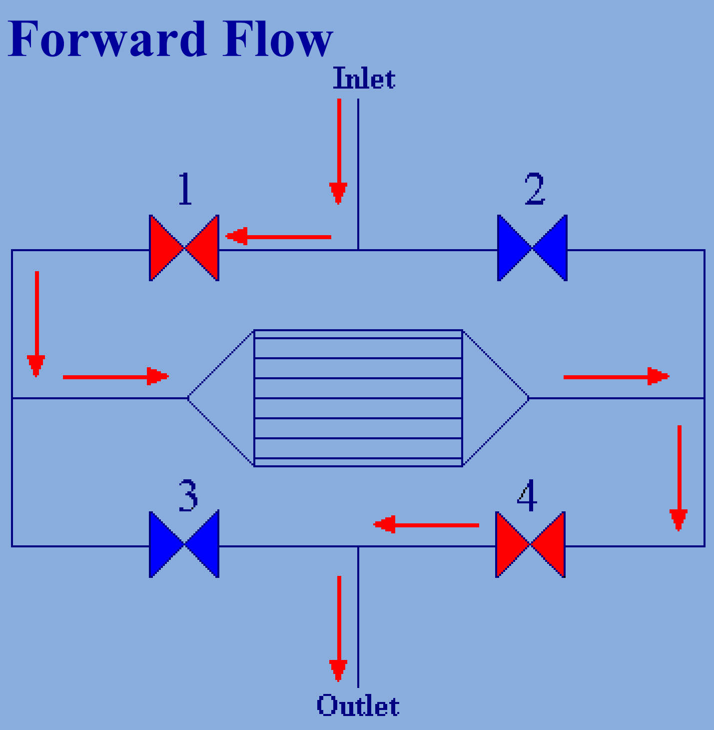


Major Obstacles

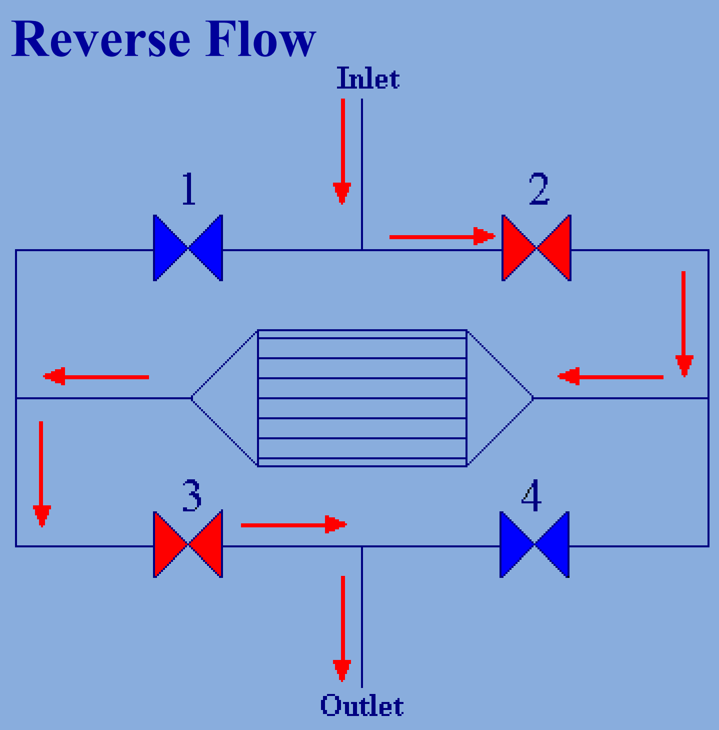
- Sulphur absorbed on NO_x trap reduces NO_x conversion efficiency
- Desulfurization process occurs at high temperature (~ 600 °C)

Reverse Flow Oxidation Catalyst Concept

For exothermic reactions reverse-flow reactor is a heat trap system which is capable of maintaining high temperatures.

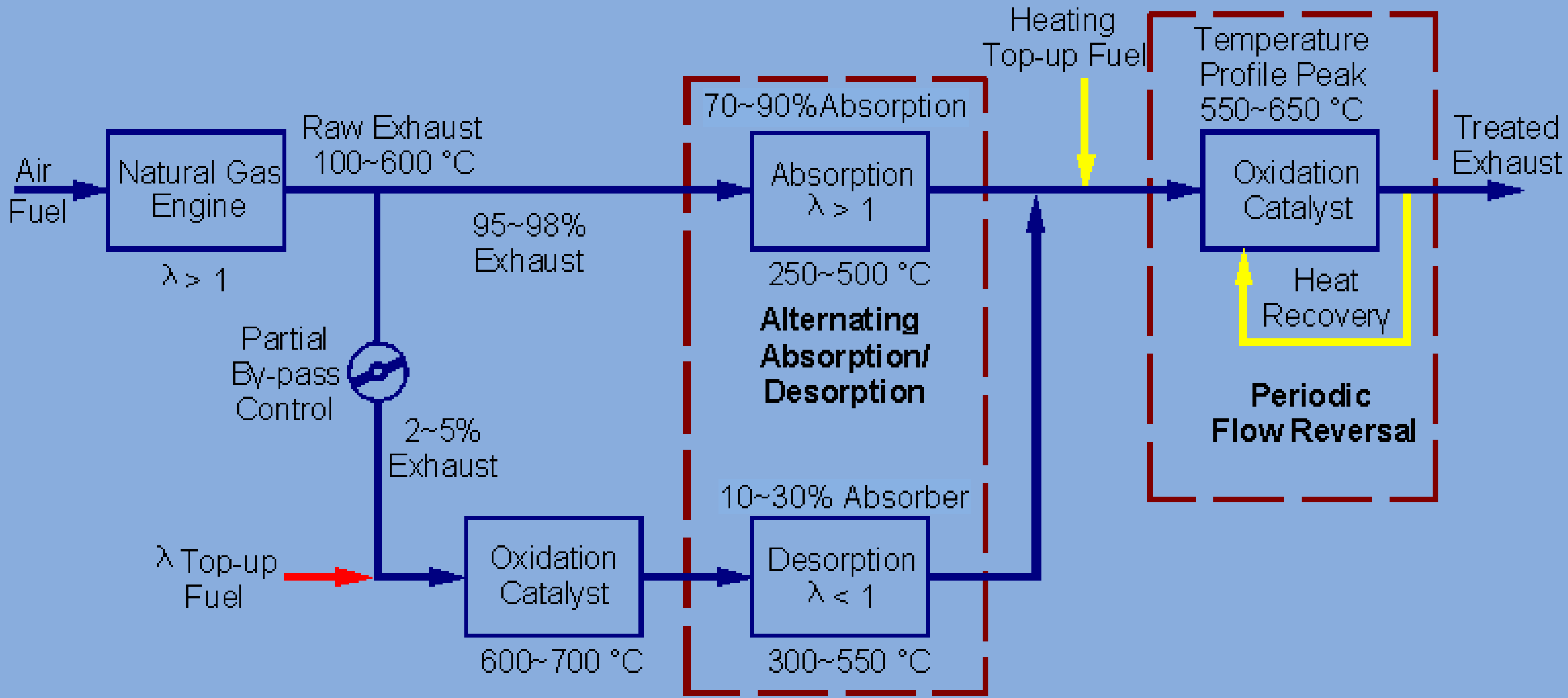


1 and 4 opened ; 2 and 3 closed



1 and 4 closed ; 2 and 3 opened

Space Shared LNT Absorption/Desorption Alternating Operation Incorporated with Flow Reversal Oxidation



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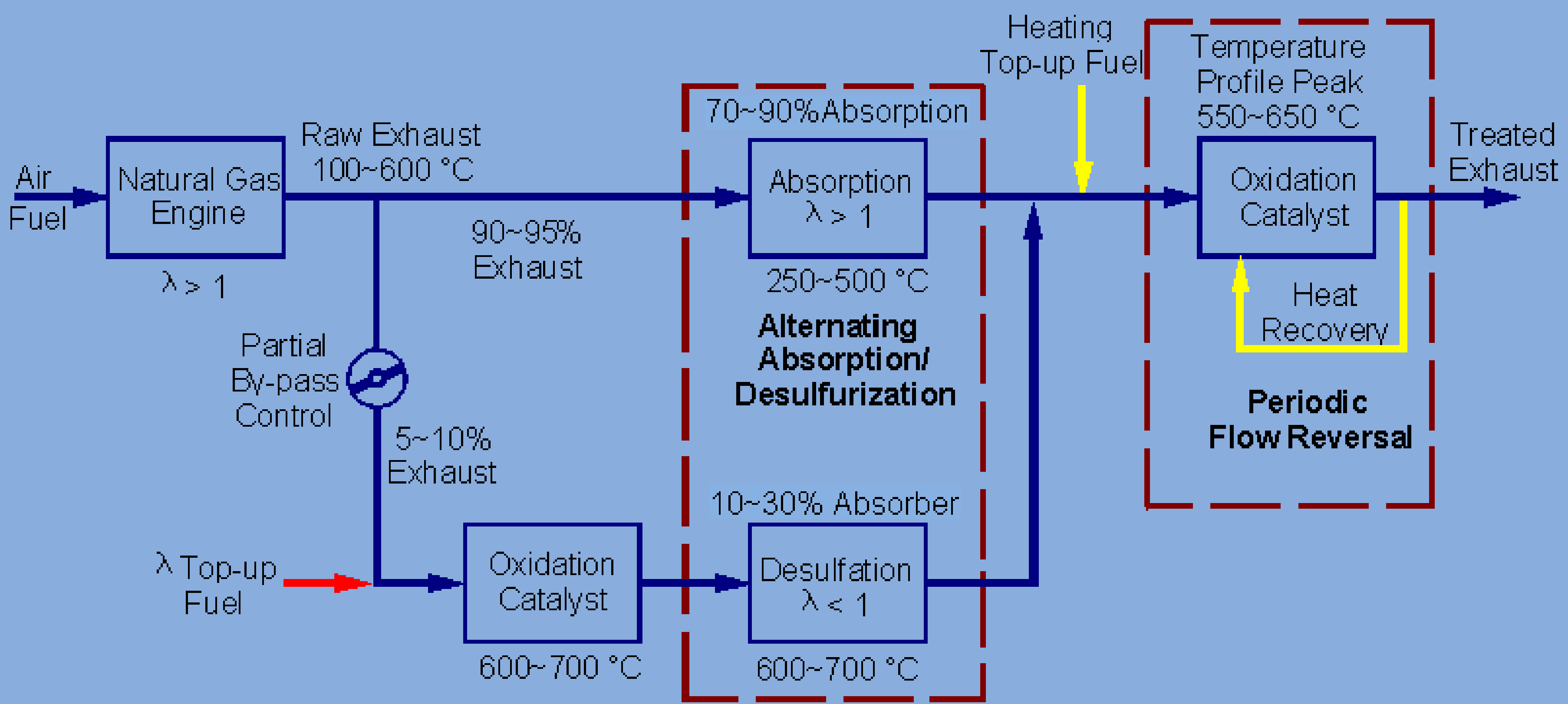


Major Issues

NO_x Absorbing Catalyst

- Frequency of regeneration and desulfurization modes
- Duration of supplemental fuel injection

Reverse-Flow Oxidation Catalyst

- Duration of supplemental fuel injection
- Switching time

These issues are resolved by performing experiments in the bench-flow reactor system

Bench-Flow Reactor

The bench-flow reactor is used to study the effects of the following parameters on the performance of NO_x absorbing and oxidation catalysts

- Space Velocity (10,000 - 100,000 hr^{-1})
- Inlet Gas Temperature (200 - 600 °C)
- Gas Composition

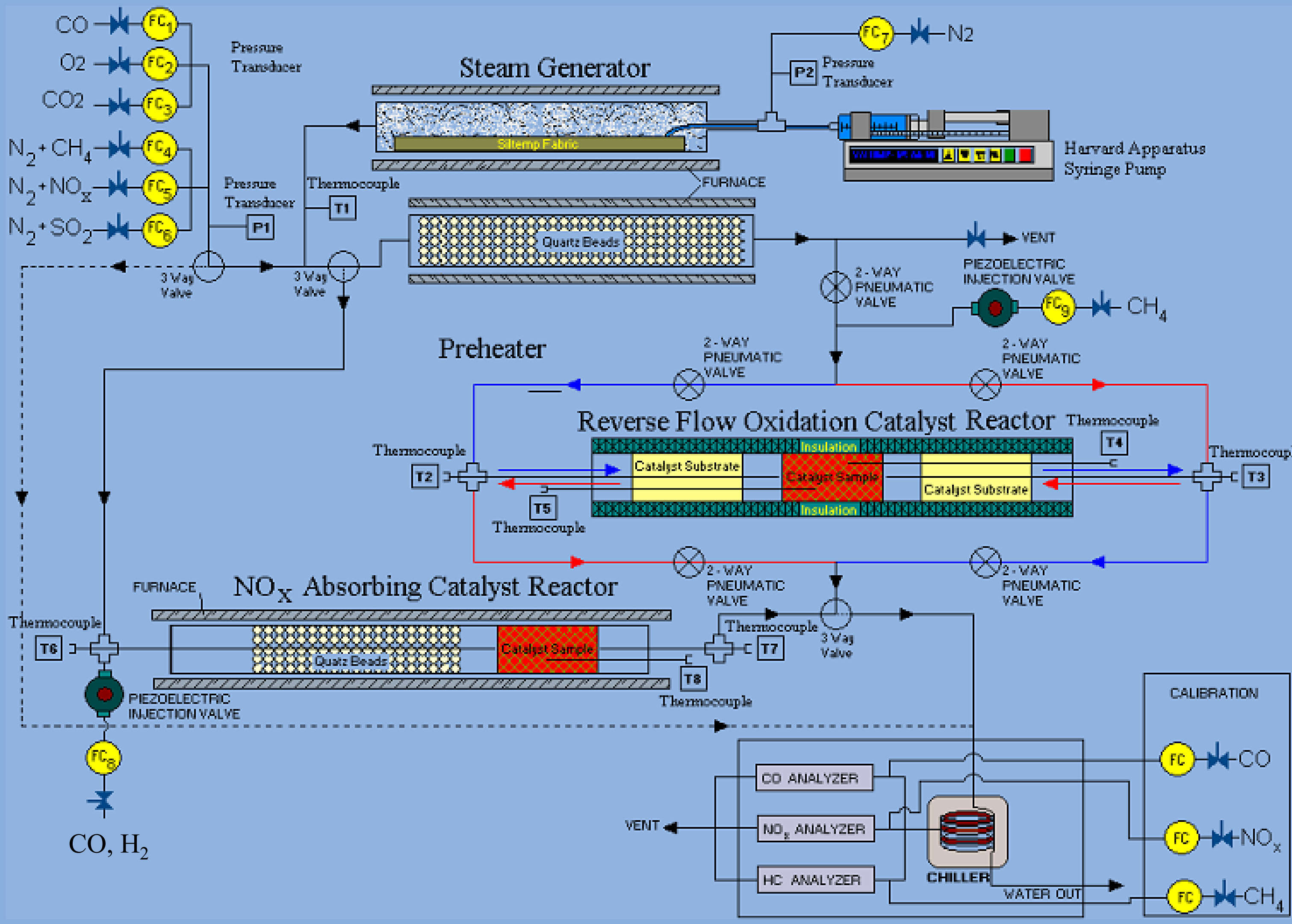
The bench flow reactor system consists of the following components

- Gas supply system
- Preheater
- NO_x absorbing catalyst reactor
- Reverse-flow oxidation catalyst reactor
- Supplemental fuel injection systems
- Analyzer system
- Labview-based data acquisition system

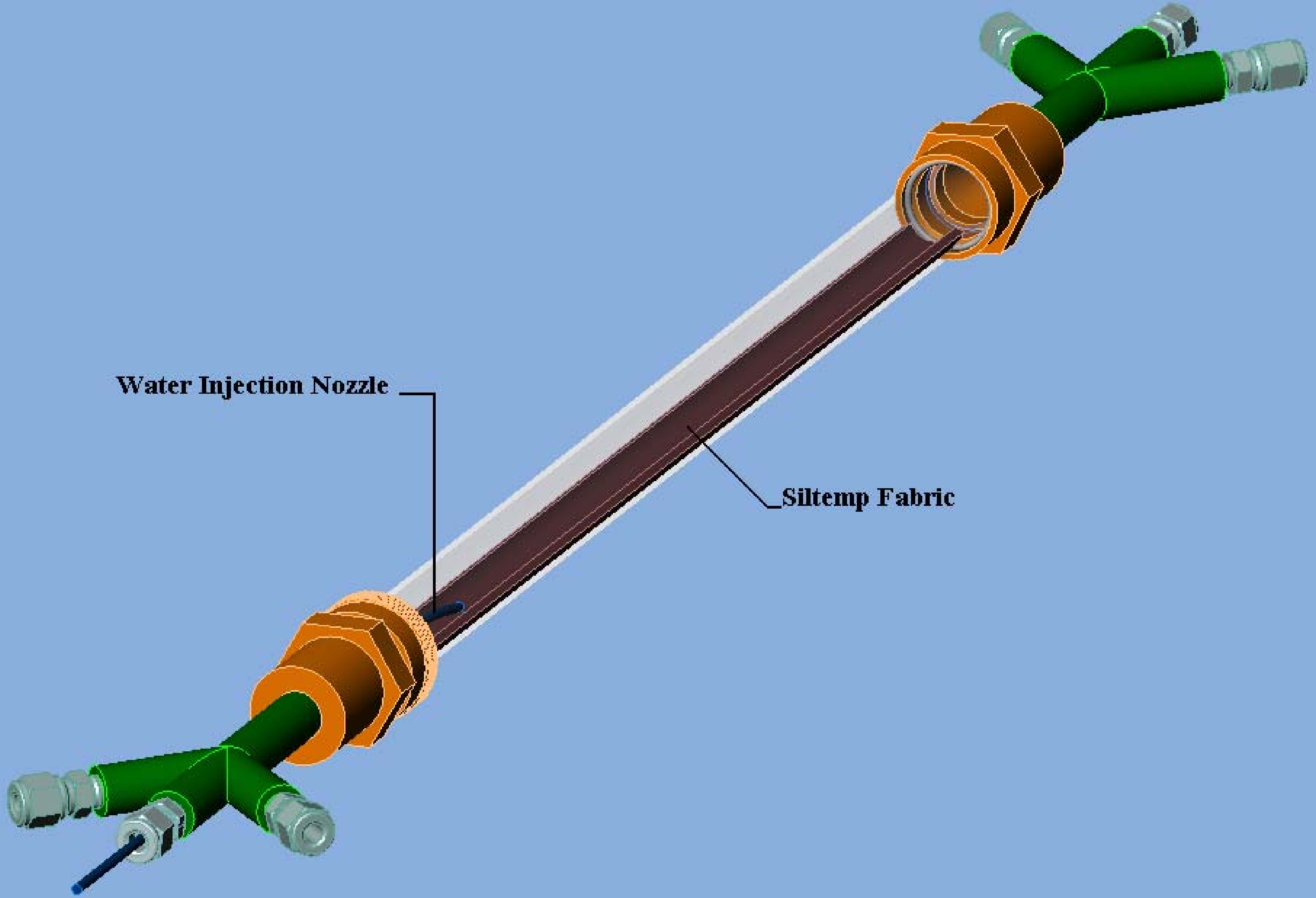
Exhaust Gas Composition

NO	1000 ppm
CO	1%
CH_4	1500 ppm
CO_2	12%
H_2O	10%
O_2	8%
N_2	Balance

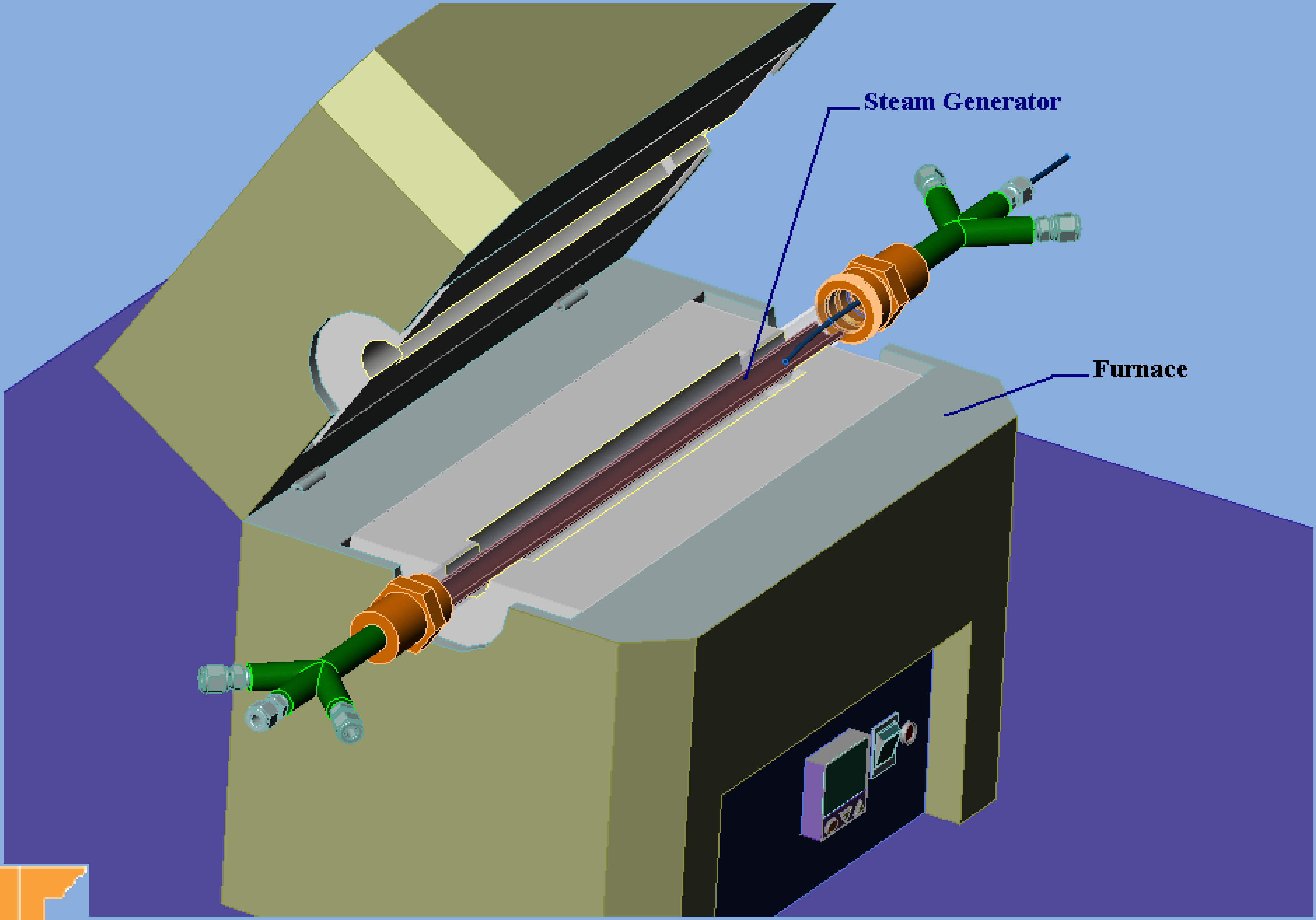
Schematic of Bench-Flow Reactor System



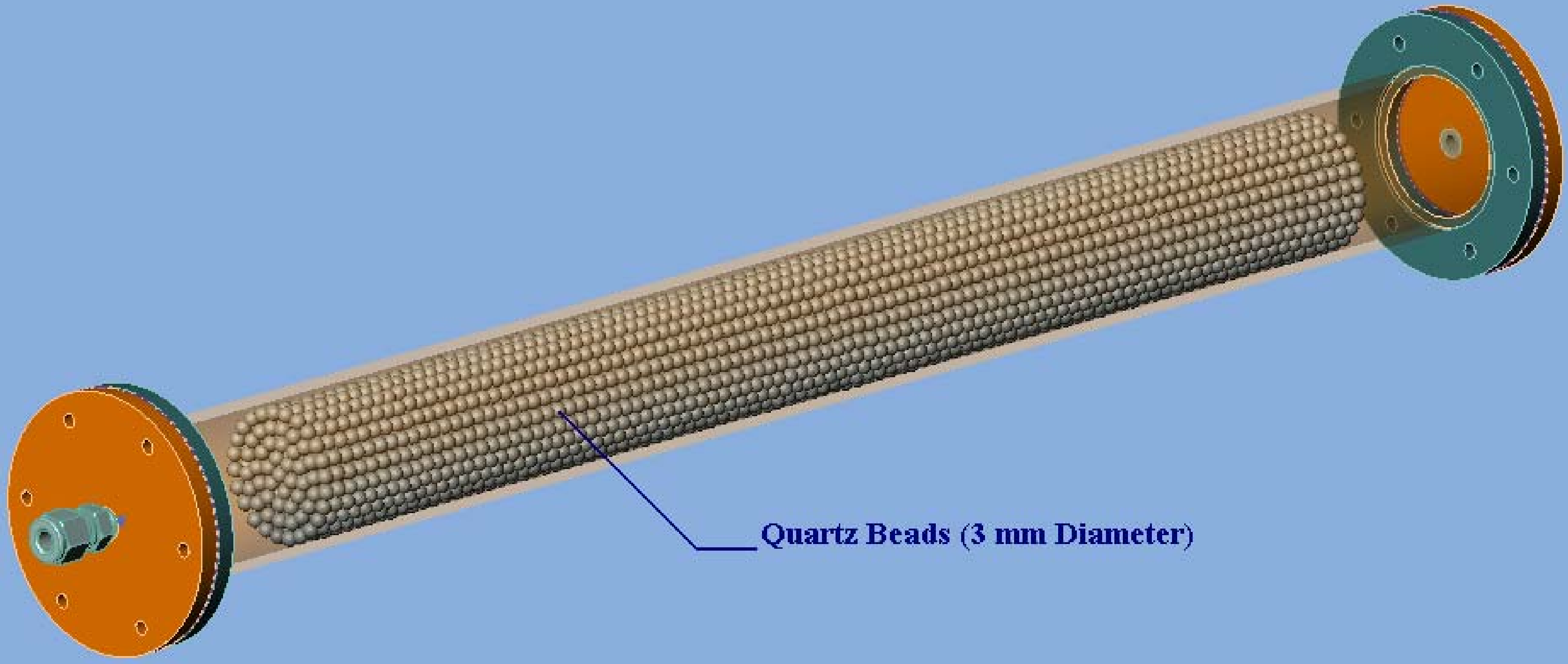
Steam Generator



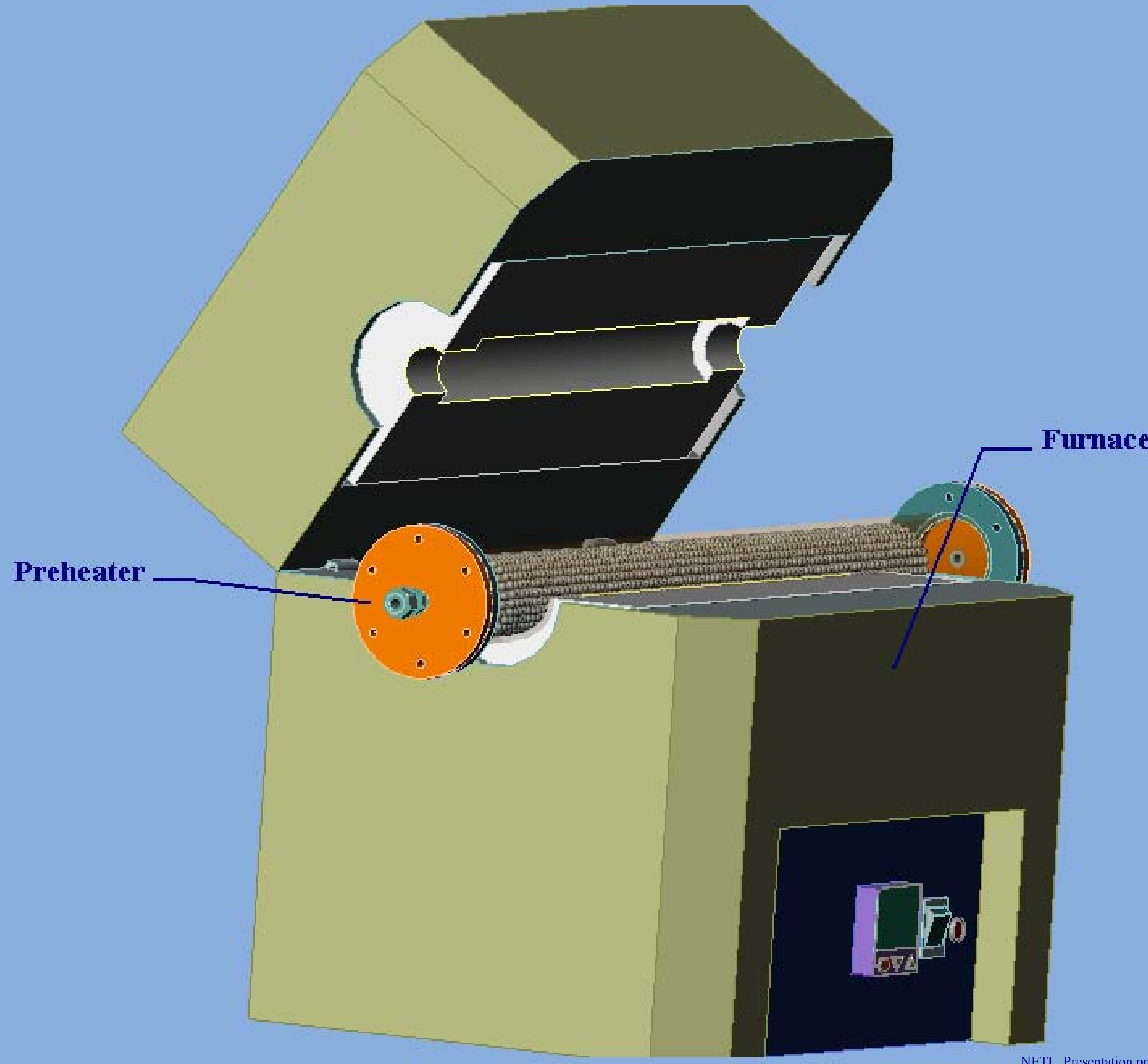
Steam Generator and Furnace



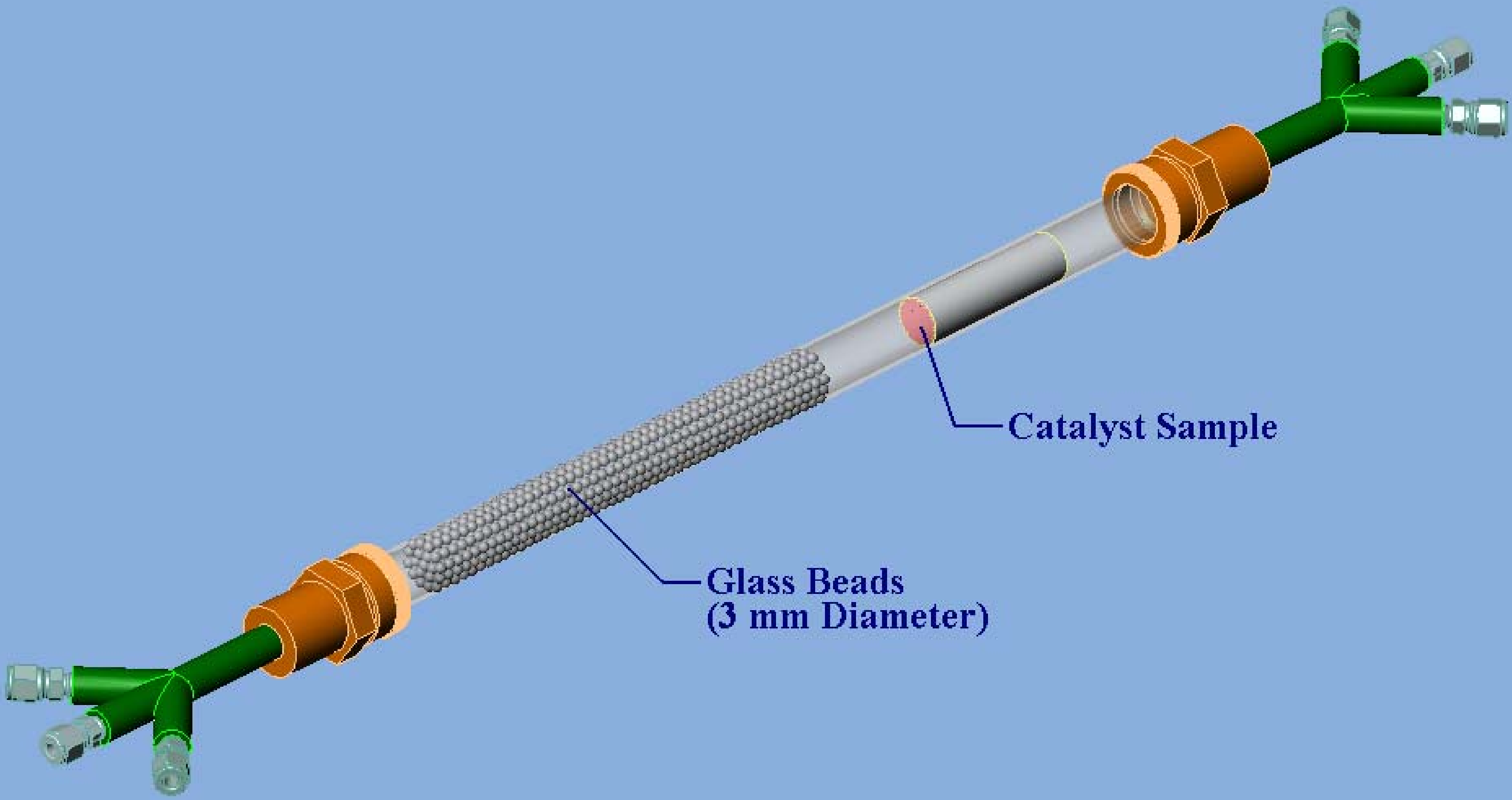
Preheater



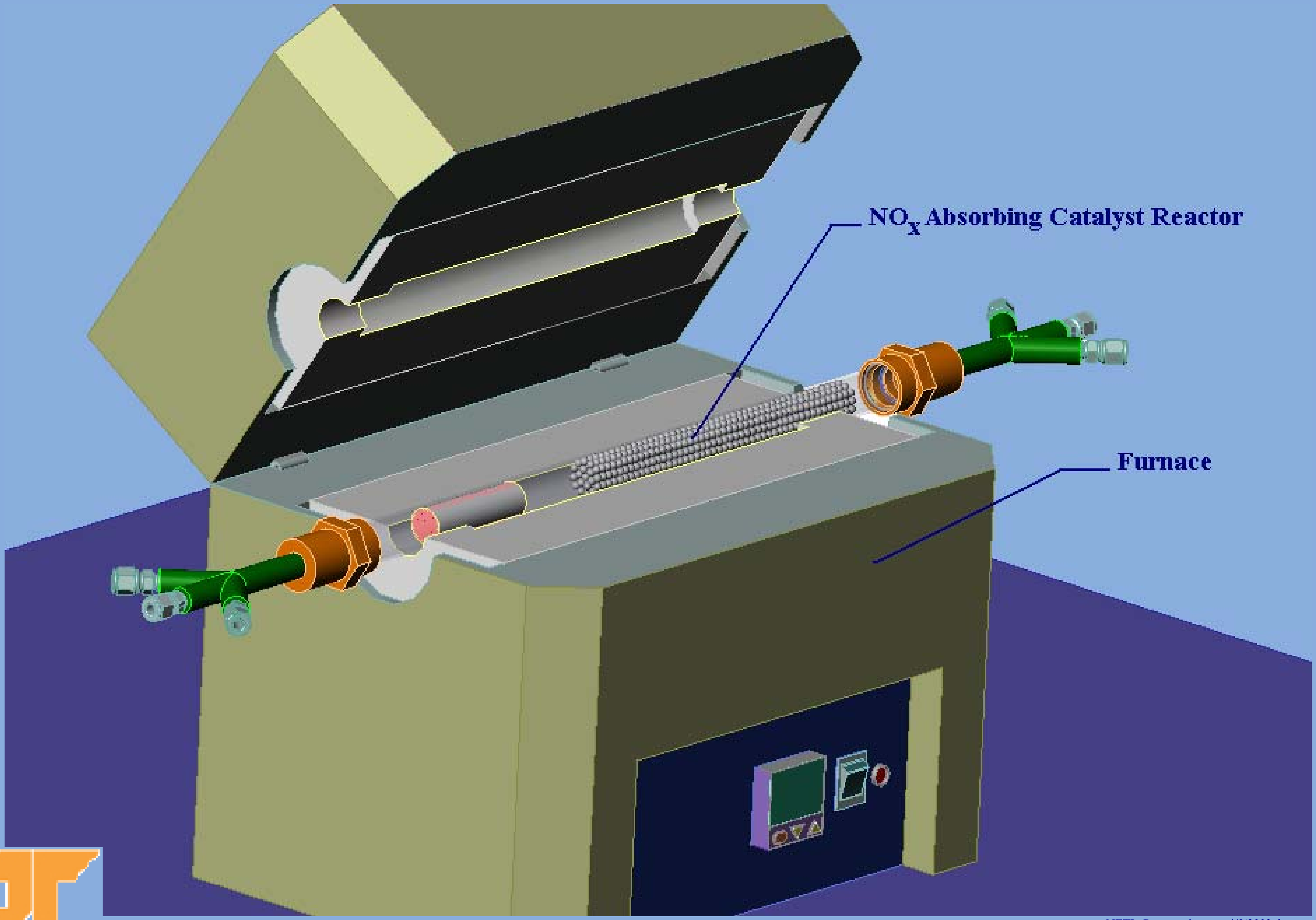
Preheater and Furnace



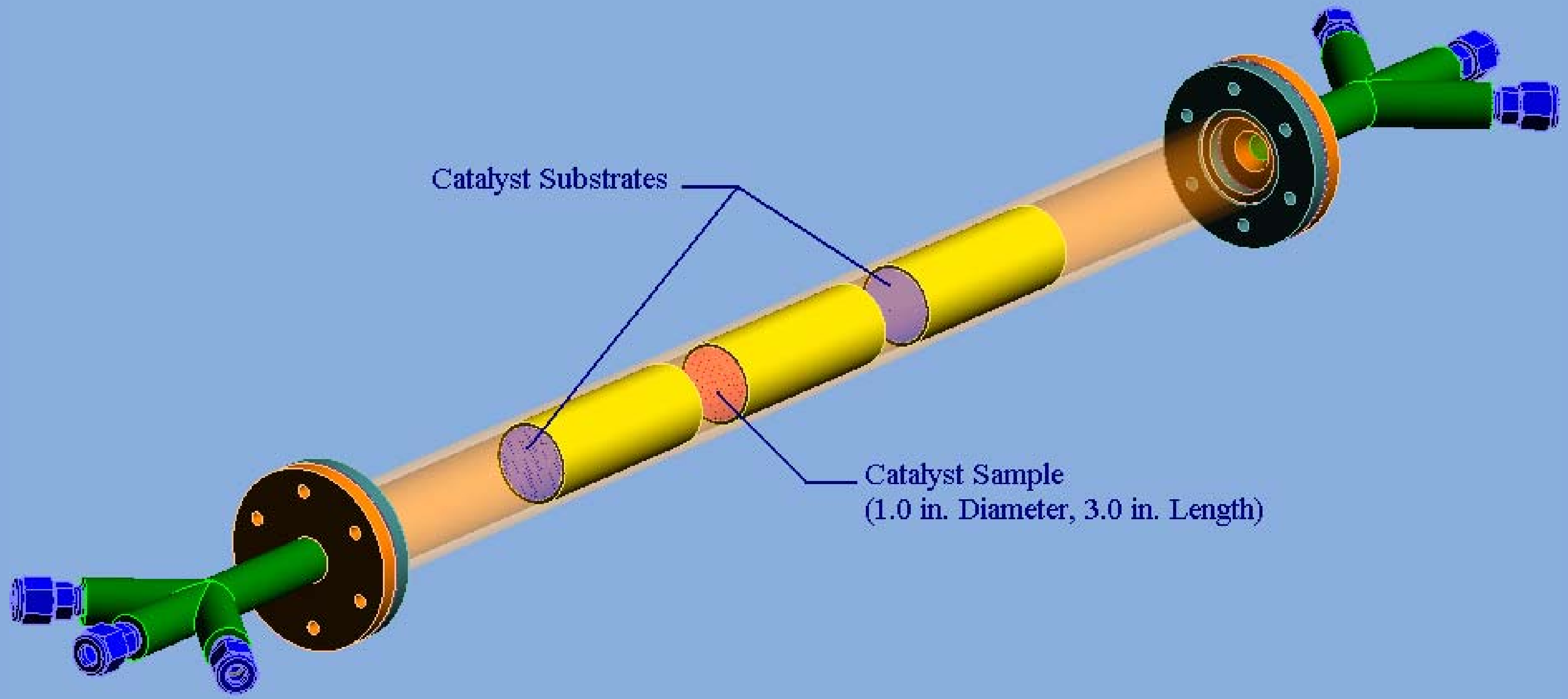
NO_x Absorbing Catalyst Reactor



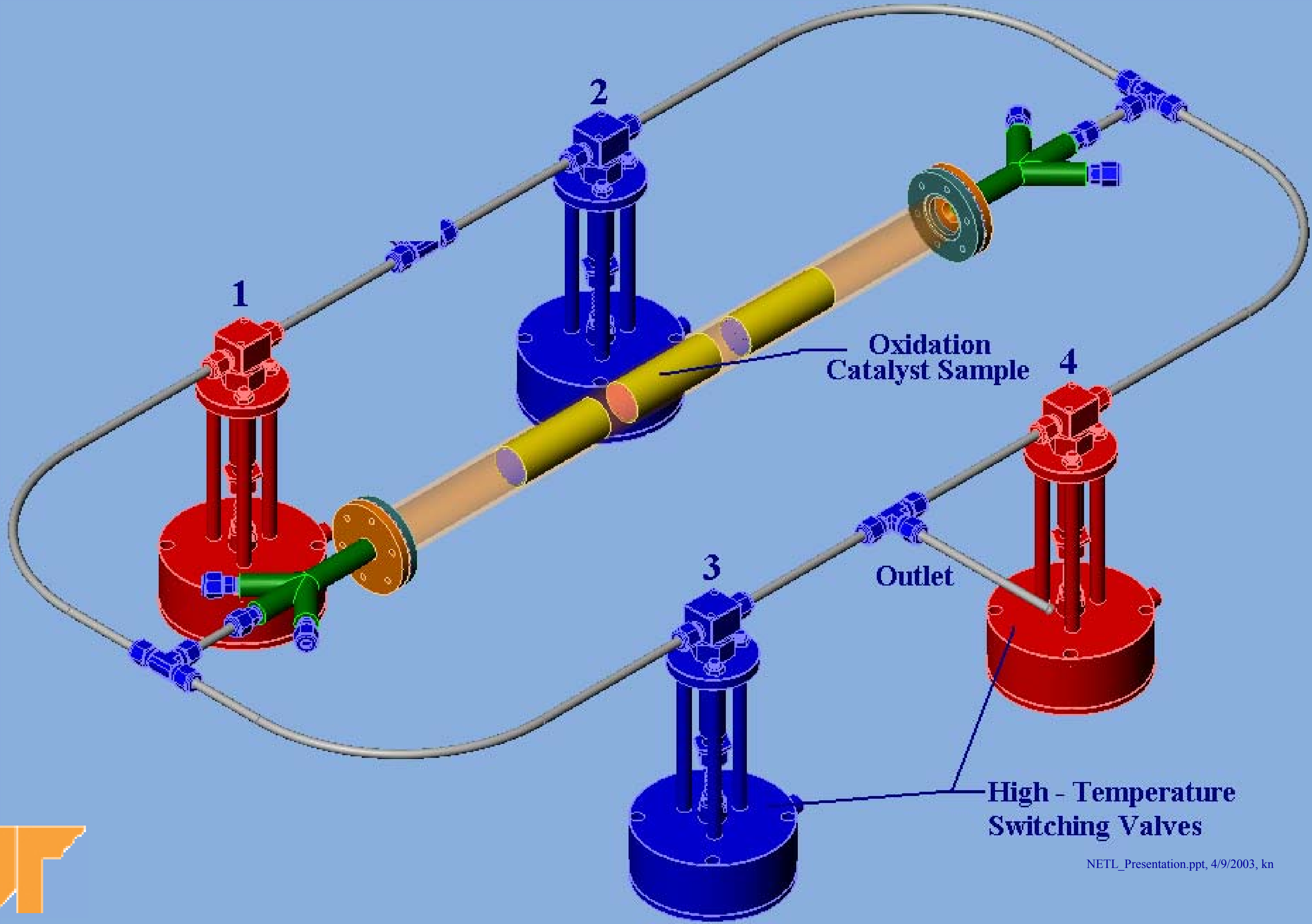
NO_x Absorbing Catalyst Reactor and Furnace



Reverse-Flow Oxidation Catalyst Reactor



Reverse-Flow Oxidation Catalyst Reactor and High Temperature Switching Valves



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Instrument Panel

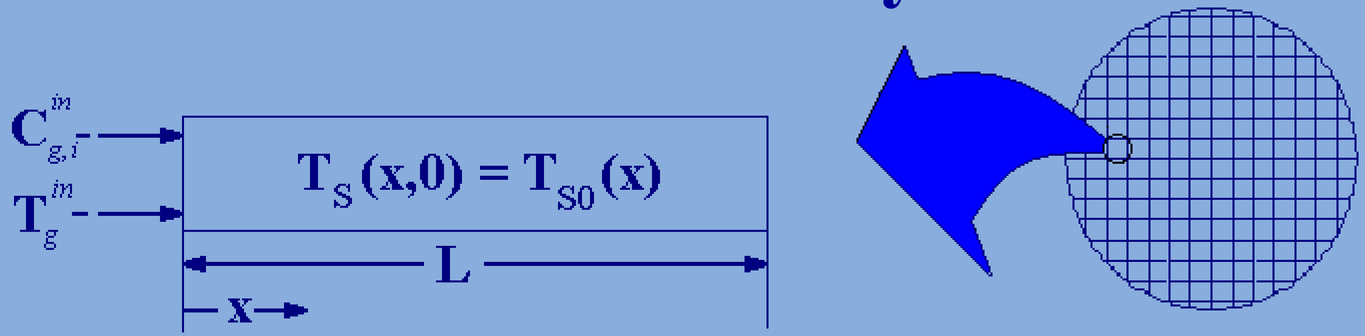
Mathematical Modeling of a Reverse-Flow Oxidation Catalyst

A transient 1-D heterogeneous plug flow model is developed for the analysis of reverse-flow oxidation catalysts. The model accounts for simultaneous processes of heat transfer, mass transfer, and chemical reactions.

The model is used to predict the effects of the following parameters on temperature profile and methane (CH_4) conversion.

- **Exhaust Gas Flow Rate**
- **Exhaust Gas Temperature**
- **Switching Time**

Mathematical Modeling of a Reverse-Flow Oxidation Catalyst



$$\frac{\partial T_S(0,t)}{\partial x} = 0 \qquad \frac{\partial T_S(L,t)}{\partial x} = 0$$

Initial Condition:

$$T_S(x,0) = T_{S0}(x)$$

Boundary Conditions:

$$C_{g,i}(0,t) = C_{g,i}^{in}$$

$$T_g(0,t) = T_g^{in}$$

$$\frac{\partial T_S(0,t)}{\partial x} = \frac{\partial T_S(L,t)}{\partial x} = 0$$

Mathematical Modeling of a Reverse-Flow Oxidation Catalyst

Assumptions:

a) All channels in the monolith are assumed to behave similarly

b) Neglect radial variations of gas-phase temperature, concentration, and velocity within the individual channels. Thermophysical properties are assumed to be constant.

c) Number of active sites is assumed constant.

d) Negligible temperature gradients in the solid phase in the transverse direction.

e) Negligible axial diffusion of mass and heat in the gas phase

f) Chemical reactions occur only on the external surface of the catalytic wall.

g) The gas is in pseudo steady state at any time with the wall temperature profile

Mathematical Modeling of a Reverse-Flow Oxidation Catalyst

Governing Equations

Material balance for gas phase:

$$\varepsilon \frac{\partial C_{g,i}}{\partial t} = -v \frac{\partial C_{g,i}}{\partial x} - k_{m,i} S (C_{g,i} - C_{s,i}) \qquad (1) \qquad i = 1, \ldots\ldots, N$$

Energy balance for gas phase:

$$\varepsilon \rho_g C_{pg} \frac{\partial T_g}{\partial t} = -v \rho_g C_{pg} \frac{\partial T_g}{\partial x} + hS(T_s - T_g) \qquad (2)$$

Material balance for solid phase:

$$a(x) R_i (C_s, T_s) = \frac{P_{tot}}{R_g T_g} k_{m,i} S (C_{g,i} - C_{s,i}) \qquad (3) \qquad i = 1, \ldots\ldots, N$$

Energy balance for solid phase:

$$(1-\varepsilon)\rho_s \frac{\partial (C_{ps} T_s)}{\partial t} = \lambda_s (1-\varepsilon) \frac{\partial^2 T_s}{\partial x^2} + hS(T_g - T_S) + a(x) \sum_{i=1}^{4} (-\Delta H)_i R_i (C_S, T_S) \qquad (4)$$

Mathematical Modeling of a Reverse-Flow Oxidation Catalyst

Reaction Kinetics:

Oxidation reactions for CO, H_2, and CH_4 over palladium are used in this model.

$$CO + (1/2)O_2 \longrightarrow CO_2$$

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_20$$

$$H_2 + (1/2)O_2 \longrightarrow H_2O$$

Mathematical Modeling of Reverse Flow Oxidation Catalyst

Nomenclature

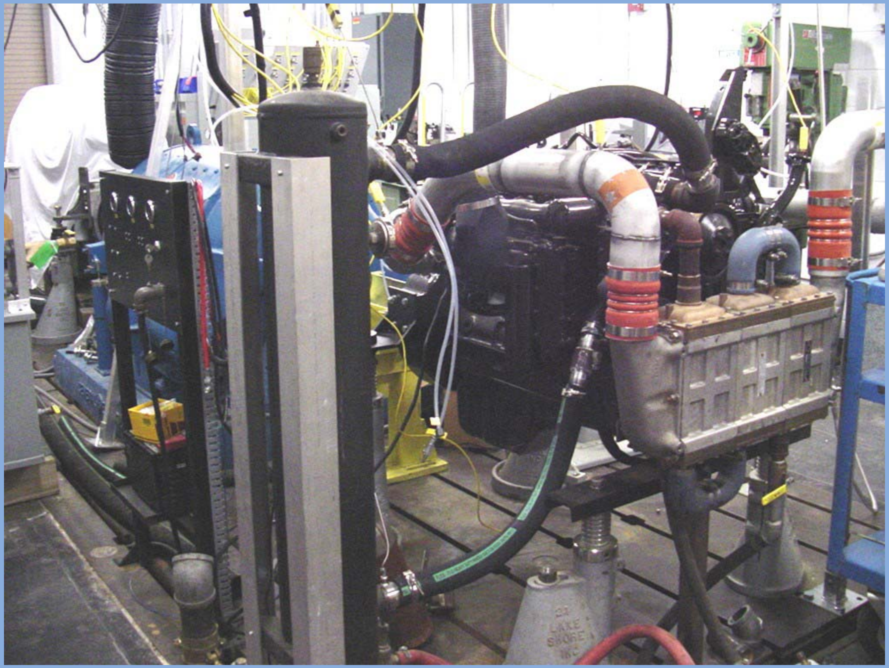
ε	Void Fraction of Monolith
ρ_g	Gas Density
$C_{g,i}$	Concentration of Specie "i" in the Bulk Stream
$k_{m,i}$	Mass Transfer Coefficient of Specie "i"
h	Convective Heat Transfer Coefficient
S	Geometric Surface Area per Unit Reactor Volume
$a(x)$	Catalytic Surface Area per Unit Reactor Volume
R_i	Specific Reaction Rate for Specie "i"
C_{ps}	Specific Heat of Solid
$C_{s,i}$	Concentration of Specie "i" at the Wall
P_{tot}	Total Pressure

Engine Test Cell

Collaboration with our colleagues at Oak Ridge National Laboratory

- Engine test cell located at National Transportation Research Center, a partnership between UTK and ORNL
- Baseline operating data for the engine and aftertreatment system to be shared between this project and ORNL's project- "NO_x Emissions Control for Natural Gas Engines and Natural Gas Vehicles"
- Aftertreatment system supplier for ORNL project will supply initial catalyst samples for bench flow reactor studies, allowing direct comparison of results
- One MS student working at NTRC in support of installation and setup of the engine, data acquisition system, and emissions analysis equipment- will also perform baseline testing

Engine Test Cell



- Cummins CG-280- installed
- 500 hp motoring DC dyno w/ shaft torque meter- operational
- California Analytic gas analyzers- bench operational
- Dyne Systems Cell Assistant Data Acquisition- operational
- Natural gas fuel system installed, procedures written, awaiting final approval from ORNL Fire Protection Engineering

Summary

Lean-Burn Natural Gas Engine and Exhaust Aftertreatment System

- Engine test cell ready for baseline testing
- Testing should begin in May after operation approval and shakedown

Bench Flow Reactor System

- System design completed
- Hardware fabricated and procured
- Assembly progressing
- Control and data acquisition system specification developed

Modeling

- Learning to use FEMLAB software

Project Team

Lean-Burn Natural Gas Engine and Exhaust Aftertreatment System

Dr. David Irick

David Smith, PhD Student

Aaron Williams, MS Student

John Miller, Undergraduate Student

Bench Flow Reactor System and Modeling

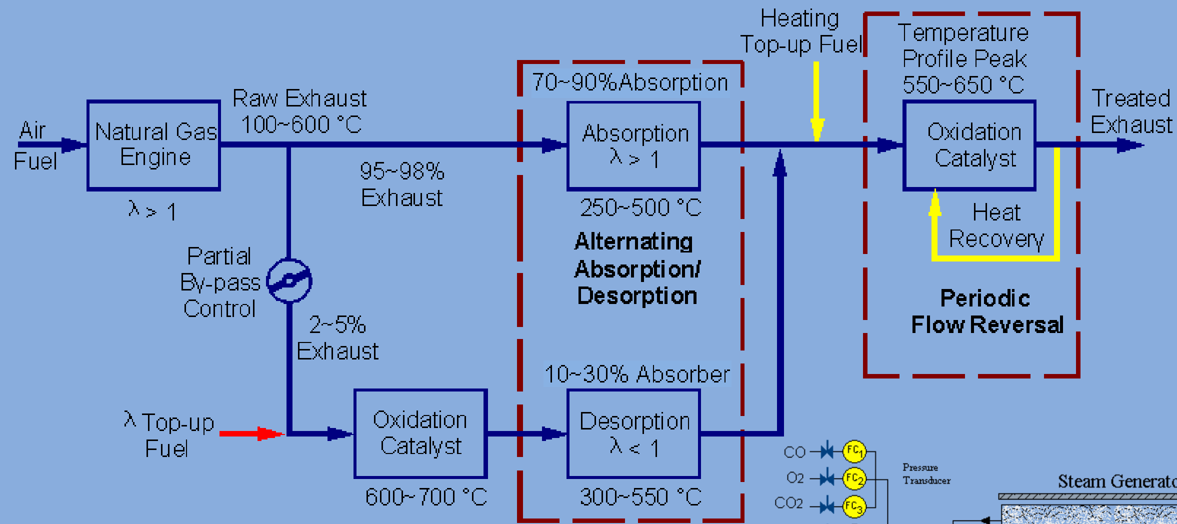
Prof. Ke Nguyen

S. Scott Smith, MS Student

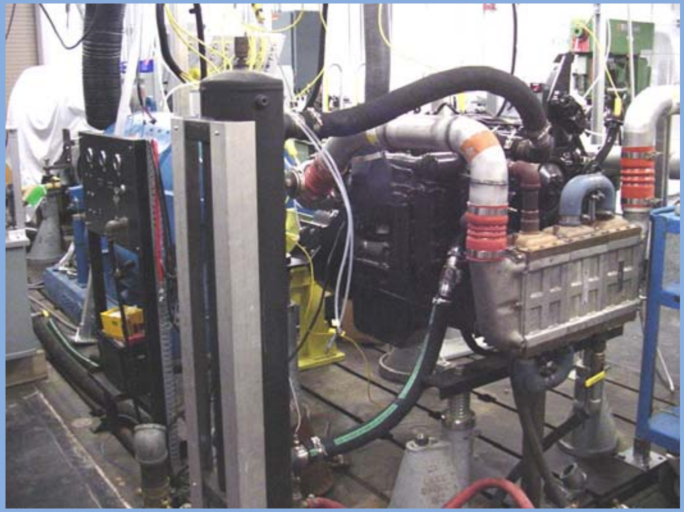
Jessica Rinaldy, MS Student

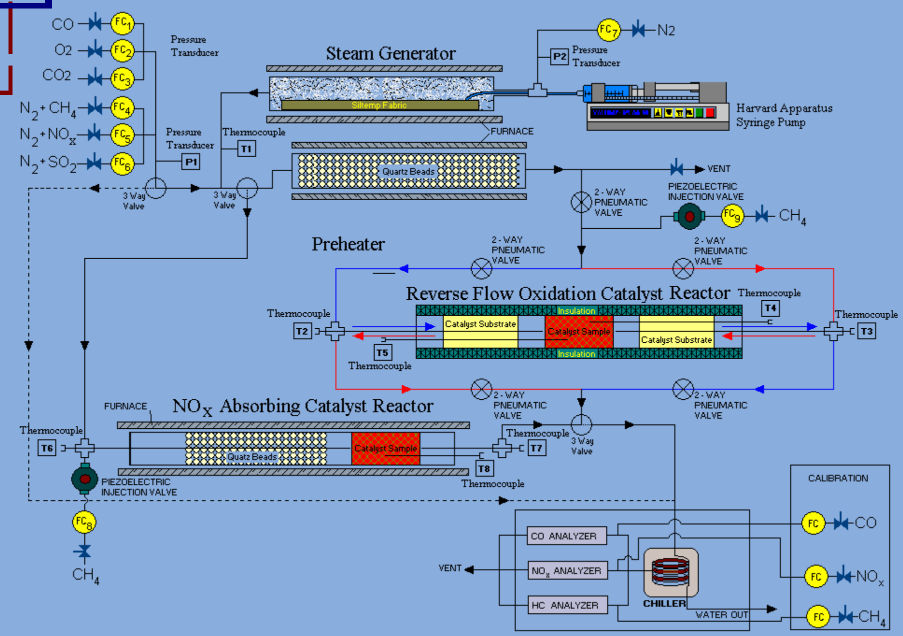
Raymond McDonnel, Undergraduate Student

Questions?



Air
Fuel
Natural Gas Engine
λ > 1
Raw Exhaust 100~600 °C
95~98% Exhaust
Partial By-pass Control
2~5% Exhaust
λ Top-up Fuel
Oxidation Catalyst
600~700 °C
70~90%Absorption
Absorption λ > 1
250~500 °C
Alternating Absorption/ Desorption
10~30% Absorber
Desorption λ < 1
300~550 °C
Heating Top-up Fuel
Temperature Profile Peak 550~650 °C
Oxidation Catalyst
Heat Recovery
Periodic Flow Reversal
Treated Exhaust





Steam Generator
Harvard Apparatus Syringe Pump
Preheater
Reverse Flow Oxidation Catalyst Reactor
NOx Absorbing Catalyst Reactor
PIEZOELECTRIC INJECTION VALVE
CO ANALYZER
NOx ANALYZER
HC ANALYZER
CHILLER
CALIBRATION
VENT
WATER OUT